Scattering Kernel of polyatomic gases

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Abstract.
This paper is devoted to the derivation of realistic laws relating the distribution functions of reflected and incoming particles at the wall. A polyatomic scattering kernel is derived using an integral operator formalism. Physically, a concept of partial accommodation was employed in the kernel derivation in agreement with different accommodation processes of the three momentum components and of the various energy modes.

1. INTRODUCTION

Realistic laws relating, at the wall, the distribution functions of incoming and reflected particles are needed as boundary condition to resolve the Boltzmann equation [1, 2, 3, 4]. Moreover, in the moderately rarefied regime these laws also allow to obtain more correct velocity slip and temperature jumps at the wall and to broaden the validity domain of the continuum approaches. In this topic, a polyatomic kernel is derived here from spectral properties of its associated integral operator using a well known scattering kernel formalism [5, 6, 3] The molecules are considered as provided with internal structure involving rotational and vibrational modes and are possibly in a strong nonequilibrium state concerning the vibrational degree of freedom.

The eigenvalues of the linear integral operator so considered depend on five parameters appearing in the kernel expression. These five parameters are shown to be equal to the accommodation coefficients of various fluxes at the wall, namely: the fluxes of the three components of momentum and the fluxes of rotational and vibrational energies of the molecules. The kernel involves a part obtained in another papers about atom-like molecules [7] and so also allows the modelling of anisotropic behaviors of reflecting surfaces. Finally, under its form completely developed the scattering kernel appears as a linear combination of 32 partial kernels describing all the possible associations of, respectively, diffuse or specular processes (according to three directions) and elastic or inelastic processes (for the internal modes). The 32 coefficients of this combination are related to the 32 different eigenvalues of the integral operator, and depend only on the five basic accommodation coefficients. As result, in addition to the interplay between the momentum components included in the kernel of unstructured molecules, the polyatomic model also allows interplay between the different energy modes. The introduction of such interplays could be a partial reply to recent criticisms recently formulated about the scattering kernel formalism [8].

2. POLYATOMIC SCATTERING KERNEL DERIVATION.

We consider the problem of finding the scattering kernel $B(V',E_{ir'},E_{iv'},g_{ir'},V,E_{ir},E_{iv},g_{ir})$ governing the reflection of polyatomic molecules at the wall. V' is the velocity of the impinging gas particle referred to the wall, $V' = (V'_x,V'_y,V'_z) \in \{\Omega' = \Omega'_x \times \Omega'_y \times \Omega'_z = \mathbf{R}_- \times \mathbf{R} \times \mathbf{R}\}$ and V the velocity of the reflected one referred to the wall, $V = (V_x,V_y,V_z) \in \{\Omega = \Omega_x \times \Omega_y \times \Omega_z = \mathbf{R}_+ \times \mathbf{R} \times \mathbf{R}\}$. These velocities reduce to the peculiar velocities when the slip velocity at the wall is neglected. V_R is defined as $V_R = (-V_x,V_y,V_z)$. (x,y,z) are the three spatial coordinates with x the normal axis to the wall oriented from the wall toward the gas. $E_{ir'}$ and $E_{iv'}$ are respectively the rotational energy and the vibrational energy of an incident particle at the wall. Similarly E_{ir} and E_{iv} are respectively the rotational energy and

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the vibrational energy of a reflected particle at the wall. Then the subscripts $_{ir}$ and $_{iv}$ are the quantum numbers related to the internal energy of a particle, hence they are integers; g_{ir} is the weight of the rotational degeneracy and will be taken here equal to $(2ir+1)$. The kernel B, which is the density of probability that a molecule in a state $(V', E_{ir'}, E_{iv'})$ hitting the wall at any point X of the wall is reflected at the same point in a state $(V, E_{ir}, E_{iv},)$, must satisfy the following conditions of non-negativity, normalization, and of reciprocity [3, 1, 2]:

$$B(V', E_{ir'}, E_{iv'}, g_{ir'}, V, E_{ir}, E_{iv}, g_{ir}) \geq 0 \ , \tag{1}$$

$$\sum_{ir,iv} \int_{\Omega} B(V', E_{ir'}, E_{iv'}, g_{ir'}, V, E_{ir}, E_{iv}, g_{ir}) dV = 1 \ , \tag{2}$$

$$\begin{aligned} |V'_x| e^{-\frac{\|V'\|^2}{C_w^2}} e^{-\varepsilon_{ir'}} e^{-\varepsilon_{iv'}} g_{ir'} B(V', E_{ir'}, E_{iv'}, V, E_{ir}, E_{iv}) = \\ V_x e^{-\frac{\|V\|^2}{C_w^2}} e^{-\varepsilon_{ir}} e^{-\varepsilon_{iv}} g_{ir} B(-V, E_{ir}, E_{iv}, -V', E_{ir'}, E_{iv'}) \ ; \end{aligned} \tag{3}$$

where ε_{ir} and ε_{iv} are the dimensionless energies : $\varepsilon_{ir} = \frac{E_{ir}}{kT_w}$, $\varepsilon_{iv} = \frac{E_{iv}}{kT_w}$, with k the Boltzmann constant and T_w the wall temperature.

2.1. Analytical derivation from integral operator

Let us write the transformation

$$\begin{aligned} K(V, E_{ir}, E_{iv}, g_{ir}, V', E_{ir'}, E_{iv'}, g_{ir'}) = [\mid V'_x \mid f_0(V', E_{ir'}, E_{iv'})]^{\frac{1}{2}} [\mid V_x \mid f_0(V, E_{ir}, E_{iv})]^{\frac{-1}{2}} \\ B(V'_R, E_{ir'}, E_{iv'}, g_{ir'}, V, E_{ir}, E_{iv}, g_{ir}) \end{aligned} \tag{4}$$

where $f_0(V, E_{ir}, E_{iv})$ is the local equilibrium distribution function at the temperature T_w of the wall, defined by:

$$f_0(V, E_{ir}, E_{iv}) = \frac{n}{(C_w\sqrt{\pi})^3} e^{-\frac{\|V\|^2}{C_w^2}} \frac{g_{ir} e^{-\varepsilon_{ir}} e^{-\varepsilon_{iv}}}{Q_r Q_v} \tag{5}$$

with

$$Q_r = \sum_{ir} g_{ir} e^{-\varepsilon_{ir}} \ , \qquad Q_v = \sum_{iv} e^{-\varepsilon_{iv}} \ , \qquad C_w^2 = \frac{2kT_w}{m} \ . \tag{6}$$

Since f_0 is a known function the problem of finding B is equivalent to finding K. The normalization condition and the non-negativity conditions on B imply obviously the same conditions on K.

Note $\mathscr{F}_r$ the set of the rotational energy states E_{ir}, and $\mathscr{F}_v$ the set of the vibrational energy states E_{iv}. Consider the five elementary Hilbert space of states $L^2(\Omega_\kappa)_{\kappa=x,y,z}$, $L^2(\mathscr{F}_r)$, and $L^2(\mathscr{F}_v)$ of square summable functions with their corresponding usual scalar product

$$\begin{array}{lcll} < \varphi_{\kappa 1}, \varphi_{\kappa 2} >_\kappa & = & \int_{\Omega_\kappa} \varphi_{\kappa 1}(V) \varphi_{\kappa 2}(V) dV \ , & \varphi_{\kappa 1}, \varphi_{\kappa 2} \in \ L^2(\Omega_\kappa) \ , \quad \kappa = x,y,z \\ < \varphi_{r1}, \varphi_{r2} >_r & = & \sum_{ir} \varphi_{r1}(E_{ir}) \varphi_{r2}(E_{ir}) \ , & \varphi_{r1}, \varphi_{r2} \in \ L^2(\mathscr{F}_r) \\ < \varphi_{v1}, \varphi_{v2} >_v & = & \sum_{iv} \varphi_{v1}(E_{iv}) \varphi_{v2}(E_{iv}) \ , & \varphi_{v1}, \varphi_{v2} \in \ L^2(\mathscr{F}_v) \end{array}$$

Consider The tensor product $\pounds = L^2(\Omega_x) \otimes L^2(\Omega_y) \otimes L^2(\Omega_z) \otimes L^2(\mathscr{F}_r) \otimes L^2(\mathscr{F}_v)$ of the five Hilbert spaces of states. let us remark that this tensor product of Hilbert space $\pounds$ is dense in the Hilbert space $\mathscr{H} = L^2(\Omega) \otimes L^2(\mathscr{F}_r) \otimes L^2(\mathscr{F}_v)$ where the scalar product is defined by

$$< \varphi_1, \varphi_2 > = \sum_{ir,iv} \int_{\Omega} \varphi_1(V, E_{ir}, E_{iv}) \varphi_2(V, E_{ir}, E_{iv}) dV \ , \qquad \varphi_1, \varphi_2 \in \ \mathscr{H} \ . \tag{7}$$

Instead of studying the problem of the kernel K, we study the linear integral associated operator A defined on $\mathscr{H}$ by

$$A(\psi) = \sum_{ir',iv'} \int_{\Omega'} K(V, E_{ir}, E_{iv}, g_{ir}, V', E_{ir'}, E_{iv'}, g_{ir'}) \psi(V', E_{ir'}, E_{iv'}, g_{ir'}) d_{V'} \tag{8}$$

Assume that the operator A has a purely discret spectrum, and assume that its eigenfunctions are all in the Hilbert space $\pounds$. The kernel K can be written on the form:

$$K = \sum_{j_x,j_y,j_z,j_r,j_v=0}^{\infty} \lambda_{j_x,j_y,j_z,j_r,j_v} \psi_{j_x}(V_x)\psi_{j_y}(V_y)\psi_{j_z}(V_z)\psi_{j_r}(E_{ir})\psi_{j_v}(E_{iv}) \tag{9}$$
$$\psi_{j_x}(V'_x)\psi_{j_y}(V'_y)\psi_{j_z}(V'_z)\psi_{j_r}(E_{ir'})\psi_{j_v}(E_{iv'})$$

where the functions $\psi_{j_x}(V_x)\psi_{j_y}(V_y)\psi_{j_z}(V_z)\psi_{j_r}(E_{ir})\psi_{j_v}(E_{iv})$ are the eigenfunctions of A with their corresponding eigenvalues $\lambda_{j_x,j_y,j_z,j_r,j_v}$. According to the non-negativity and the normalization conditions, the eigenvalues must satisfy $\lambda_{j_x,j_y,j_z,j_r,j_v} \in [0,1]$ for all $j_x, j_y, j_z, j_r, j_v \in \mathbf{N}$. Moreover, one can see that, on the tensor product space $\pounds$, the scalar product (7) equals the scalar product defined on this tensor product space $\pounds$ by the product of the five elementary scalar products (7). So, we can suppose that the eigenvalues have the form $\lambda_{j_x}\lambda_{j_y}\lambda_{j_z}\lambda_{j_r}\lambda_{j_v}$ and that the set of functions $\psi_{j_\chi}(M_\chi)$, $j_\chi \in \mathbf{N}$, is a function basis of the χ corresponding Hilbert space, $\chi = x,y,z,r,v$. Therefore, the expression (9) can be written as a product of five infinite sums:

$$K = \prod_{\chi\in\{x,y,z,r,v\}} \sum_{j=0}^{\infty} \lambda_{j_\chi} \psi_{j_\chi}(M_\chi)\psi_{j_\chi}(M'_\chi) \quad , \quad M_\chi = V_x, V_y, V_z, E_{ir}, E_{iv} \ . \tag{10}$$

Define $\psi_0 = \psi_{0_x}\psi_{0_y}\psi_{0_z}\psi_{0_r}\psi_{0_v}$ by

$$\psi_{0_x}(V_x) = \frac{\sqrt{2}}{C_w} \mid V_x \mid^{\frac{1}{2}} e^{\frac{-V_x^2}{2C_w^2}} \ , \qquad \psi_{0_y}(V_y) = (C_w\sqrt{\pi})^{\frac{-1}{2}} e^{\frac{-V_y^2}{2C_w^2}} \ ,$$
$$\psi_{0_z}(V_z) = (C_w\sqrt{\pi})^{\frac{-1}{2}} e^{\frac{-V_z^2}{2C_w^2}} \ , \qquad \psi_{0_r}(E_{ir}) = \sqrt{\frac{g_{ir}}{Q_r}} e^{-\frac{1}{2}\varepsilon_{ir}} \ , \qquad \psi_{0_v}(E_{iv}) = \frac{e^{-\frac{1}{2}\varepsilon_{iv}}}{\sqrt{Q_v}} \ .$$

Let us prove that ψ_0, is an eigenfunction of A. Mathematically, the normalisation condition can be also written

$$\sum_{ir',iv'} \int_{\Omega'} B(-V, E_{ir}, E_{iv}, g_{ir}, -V'_R, E_{ir'}, E_{iv'}, g_{ir'}) d_{V'} = 1 \ , \tag{11}$$

from this relation (11), the reciprocity relation (3) leads to:

$$\sum_{ir',iv'} \int_{\Omega'} \mid V'_x \mid f_0(V', E_{ir'}, E_{iv'}) B(V'_R, E_{ir'}, E_{iv'}, g_{ir'}, V, E_{ir}, E_{iv}, g_{ir}) d_{V'} = \mid V_x \mid f_0(-V, E_{ir}, E_{iv}) \ . \tag{12}$$

Using the relation (12), the calculation of $A(\psi_0)$ gives $A(\psi_0) = \psi_0$. Consequently $\psi_0 = \psi_{0_x}\psi_{0_y}\psi_{0_z}\psi_{0_r}\psi_{0_v}$ is an eigenfunction of the operator A associated to the eigenvalue 1.

Now, following the five microscopic state parameters, let us introduce five parameters related to the eigenvalues as follows: $\lambda_{0_\chi} = 1$, and for $j \neq 0$, $\lambda_{j_\chi} = (1-\alpha_\chi)$ for all $\chi = x,y,z,r,v$. The relation (10) becomes

$$K = \prod_{\chi\in\{x,y,z,r,v\}} [\psi_{0_\chi}(M_\chi)\psi_{0_\chi}(M'_\chi) + (1-\alpha_\chi) \sum_{j=1}^{\infty} \psi_{j_\chi}(M_\chi)\psi_{j_\chi}(M'_\chi)] \tag{13}$$

which may be written

$$K = \prod_{\chi\in\{x,y,z,r,v\}} [\alpha_\chi \psi_{0_\chi}(M_\chi)\psi_{0_\chi}(M'_\chi) + (1-\alpha_\chi) \sum_{j=0}^{\infty} \psi_{j_\chi}(M_\chi)\psi_{j_\chi}(M'_\chi)] \ . \tag{14}$$

Finally, using the following property

$$\sum_{j=0}^{\infty} \psi_{j_\chi}(M_\chi)\psi_{j_\chi}(M'_\chi) = \delta(M_\chi - M'_\chi) \ . \tag{15}$$

where δ is the dirac function, it is obtained

$$K = \{\alpha_x \psi_{0_x}(V_x)\psi_{0_x}(V_x') + (1-\alpha_x)\delta(V_x - V_x')\}\{\alpha_y \psi_{0_y}(V_y)\psi_{0_y}(V_y') + (1-\alpha_y)\delta(V_y - V_y')\} \quad (16)$$
$$\{\alpha_z \psi_{0_z}(V_z)\psi_{0_z}(V_z') + (1-\alpha_z)\delta(V_z - V_z')\}\{\alpha_r \psi_{0_r}(V_r)\psi_{0_r}(V_r') + (1-\alpha_r)\delta(V_r - V_r')\}$$
$$\{\alpha_v \psi_{0_v}(V_v)\psi_{0_v}(V_v') + (1-\alpha_v)\delta(V_v - V_v')\} .$$

Applying inversely the transformation (4), the operator B corresponding to the kernel K above (relationship (16)) is

$$B(V', E_{ir'}, E_{iv'}, g_{ir'}, V, E_{ir}, E_{iv}, g_{ir}) = \{(1-\alpha_x)\delta(V_x' + V_x) + \alpha_x \frac{2V_x}{C_w^2} e^{-\frac{V_x^2}{C_w^2}}\} \quad (17)$$
$$\{(1-\alpha_y)\delta(V_y' - V_y) + \alpha_y \frac{1}{C_w\sqrt{\pi}} e^{-\frac{V_y^2}{C_w^2}}\}\{(1-\alpha_y)\delta(V_z' - V_z) + \alpha_z \frac{1}{C_w\sqrt{\pi}} e^{-\frac{V_z^2}{C_w^2}}\}$$
$$\{(1-\alpha_r)\delta(E_{ir'} - E_{ir}) + \alpha_r \frac{g_{ir}}{Q_r} e^{-\varepsilon_{ir}}\}\{(1-\alpha_v)\delta(E_{iv'} - E_{iv}) + \alpha_v \frac{1}{Q_v} e^{-\varepsilon_{iv}}\} .$$

In the further calculations, we will note the scattering kernel (17) simply

$$B = P_x P_y P_z P_r P_v$$

where P_x, P_y, P_z, P_r, P_v corresponds respectively to the five factors of the expression (17). It would be seen that these five factors satisfy

$$\int_0^{+\infty} P_x dV_x = \int_{-\infty}^{+\infty} P_y dV_y = \int_{-\infty}^{+\infty} P_z dV_z = \sum_{ir} P_r = \sum_{iv} P_v = 1 . \quad (18)$$

On the other hand when developing the expression (17) one obtains the kernel B as combination of 32 elementary kernels where the coefficients are functions of the α_χ.

2.2. On the coefficient α_χ

In this section we prove that the five coefficients α_χ involved in the scattering kernel equal respectively the accommodation coefficients of the various fluxes of the five microscopic state parameters ($M_\chi = V_x, V_y, V_z, E_{ir}, E_{iv}$).

The accommodation coefficient β_χ of a physical property M_χ at the wall is defined through the relation [3**?**]:

$$\beta_\chi = \frac{\Phi_\chi^- - \Phi_\chi^+}{\Phi_\chi^- - \Phi_\chi^e} . \quad (19)$$

where Φ_χ^- is the incoming flux at the wall of the property M_χ, Φ_χ^+ is the corresponding reflected flux, and Φ_χ^e is the reflected flux in the hypothetical situation of perfect accommodation to the wall. These various fluxes are written:

$$\Phi_\chi^- = \sum_{ir', iv'} \int_{\Omega'} m|V_x'| M_\chi' f^-(V', E_{ir'}, E_{iv'}, g_{ir'}) dV' \quad (20)$$

$$\Phi_\chi^+ = \sum_{ir, iv} \int_{\Omega} m|V_x| M_\chi f^+(V, E_{ir}, E_{iv}, g_{ir}) dV \quad (21)$$

where f^- and f^+ are respectively the incident and the reflected distribution functions linked by the relation

$$|V_x| f_i^+(V, E_{ir}, g_{ir}, E_{iv}) =$$
$$\sum_{ir', iv'} \int_{\Omega'} |V_x'| f^-(V', E_{ir'}, g_{ir'}, E_{iv'}) B(V', E_{ir'}, g_{ir'}, E_{iv'}, V, E_{ir}, g_{ir}, E_{iv}) dV' . \quad (22)$$

Accounting for (22), the reflected flux Φ_χ^+ (expression (21))may be rewritten:

$$\Phi_\chi^+ = \sum_{ir',iv'} \int_{\Omega'} m \mid V_x' \mid f^-(V', E_{ir'}, g_{ir'}, E_{iv'}) [\sum_{ir,iv} \int_\Omega M_\chi P_x P_y P_z P_r P_v d_V] d_{V'} \tag{23}$$

and the reflected flux in the case of perfect accommodation is written

$$\Phi_\chi^e = \sum_{ir',iv'} \int_{\Omega'} m \mid V_x' \mid f^-(V', E_{ir'}, g_{ir'}, E_{iv'}) [\sum_{ir,iv} \int_\Omega M_\chi B_e d_V] d_{V'} \tag{24}$$

where B_e the perfect accommodation scattering kernel is defined by

$$B_e = \frac{2 g_{ir}}{Q_r Q_v C_w^4 \pi} V_x e^{-\frac{\|V\|^2}{C_w^2}} e^{-\varepsilon_{ir}} e^{-\varepsilon_{iv}} \tag{25}$$

2.2.1. calculation of β_x

The normal accommodation coefficient is obtained by substituting $M_\chi = \mid V_x \mid$ in the definition (19). In this case, accounting for the property (18) and the expression of the partial operator P_x it is obtained

$$\sum_{ir,iv} \int_\Omega \mid V_x \mid P_x P_y P_z P_r P_v d_V = -(1-\alpha_x) V_x' + \alpha_x \frac{C_w \sqrt{\pi}}{2}$$

then the expression (23) yields

$$\Phi_x^+ - \Phi_x^- = \alpha_x \sum_{ir',iv'} \int_{\Omega'} m |V_x'| f^-(V', E_{ir'}, E_{iv'}, g_{ir'}) (V_x' + \frac{C_w \sqrt{\pi}}{2}) d_{V'} \ .$$

The calculation of Φ^e leads easily to

$$\Phi_x^e - \Phi_x^- = \sum_{ir',iv'} \int_{\Omega'} m |V_x'| f^-(V', E_{ir'}, E_{iv'}, g_{ir'}) (V_x' + \frac{C_w \sqrt{\pi}}{2}) d_{V'} \ .$$

Consequently we obtained from the relation (19) $\beta_x = \alpha_x$

2.2.2. calculation of β_y and β_z

The tangential accommodation coefficient, β_y is obtained by substituting $M_\chi = V_y$ in the definition relation (19). In this case it is easily seen that $\Phi_y^e = 0$. Then accounting for the property (18) the calculation of expression (23) leads to $\beta_y = \alpha_y$. Similarly it is found $\beta_z = \alpha_z$.

2.2.3. calculation of β_r and β_v

Now substitute $M_\chi = g_{ir} E_{ir}$ in the relation (19). Accounting for the property (18) it is obtained

$$\sum_{ir,iv} \int_\Omega g_{ir} E_{ir} P_x P_y P_z P_r P_v d_V = \sum_{ir} g_{ir} E_{ir} P_r = (1-\alpha_r) g_{ir'} E_{ir'} + \alpha_r \frac{Q_r^*}{Q_r}$$

where we have noted

$$Q_r^* = \sum_{ir} g_{ir}^2 E_{ir} e^{-\varepsilon_{ir}} \ .$$

Then the expression of Φ^+ leads to

$$\Phi^-_{E_{ir}} - \Phi^e_{E_{ir}} = \alpha_r \sum_{ir',iv'} \int_{\Omega'} m|V'_x| f^-(V', E_{ir'}, E_{iv'}, g_{ir'})(g_{ir'} E_{ir'} - \frac{Q^*_r}{Q_r}) d_{V'} \ .$$

Using the expression (25) of B_e, we obtain

$$\sum_{ir,iv} \int_{\Omega} g_{ir} E_{ir} B_e d_V = \frac{Q^*_r}{Q_r}$$

and then

$$\Phi^-_{E_{ir}} - \Phi^e_{E_{ir}} = \sum_{ir',iv'} \int_{\Omega'} m|V'_x| f^-(V', E_{ir'}, E_{iv'}, g_{ir'})(g_{ir'} E_{ir'} - \frac{Q^*_r}{Q_r}) d_{V'}$$

consequently, $\beta_r = \alpha_r$. In the same way, substituting $M_\chi = E_{iv}$, it is found $\beta_v = \alpha_v$. In conclusion, the five parameters α_χ involved in the scattering kernel (17) are the accommodation coefficient corresponding to the five state parameters, namely the three momentum components and the two internal energy degrees.

3. CONCLUDING REMARKS

Under its factorized form (17), the proposed scattering kernel is easy to use in the analytical calculations or to implement in numerical modelling, notably because of its simple factorized form where the incoming molecule parameters appear only through Dirac functions. In order to show its physical meaning, the expression (17) may be developed. Under its developed form, the scattering kernel appears as a linear combination of 32 elementary scattering kernels. All these elementary kernels correspond to various situations of accommodation at the wall [7]. The linear combination coefficients which represent the weight of the various types of accommodation in the reflection process are combinations of the factors α_χ and $(1-\alpha_\chi)$. In each elementary kernel each molecules states accommodates independently from the others. So the new kernel allows to take into account the interplay between the molecule freedom degrees when interacting at the wall [8]. Finally, the proposed scattering kernel appears as a complete construction based on the five accommodation coefficients corresponding to the five microscopic parameters defining the state of the molecules.

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